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6. AUTHOR(S)
Bruce M. Boghosian

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Center for Computational Science
Boston University
3 Cummington St.
Boston, MA 02215

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This document is the final report for AFOSR grant F49620-95-1-0285, "The Dynamics of Correlations in Lattice Gases." Under the terms of this grant, the Center for Computational Science at Boston University provided theoretical and computational support to the Lattice-Gas Theory and Computation group at the Geophysics Directorate of Phillips Laboratory (AFOSR task 2304CP). Twelve publications have resulted from this effort, as well as the sponsorship of the Sixth International Conference on Discrete Models for Fluid Mechanics, and the preparation of the proceedings of that meeting as a special issue of the International Journal of Modern Physics C. In addition to applying lattice-gas algorithms to systems of complex fluids and droplets, the work has resulted in two significant extensions of the lattice-gas algorithm: These are integer lattice gases which are proving to be an important methodology for the matching of microscopic, particulate, kinetic descriptions to macroscopic, continuum hydrodynamics, and quantum lattice gases which provide a paradigm for the simulation of physical systems on quantum computers. Moreover, we have shown that lattice-gas algorithms can be among the most efficient methods of simulating certain systems of interest in materials science, such as immiscible and amphiphilic fluids.

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An Overview of the Lattice-Gas Research Collaboration Between the Boston University Center for Computational Science and the Geophysics Directorate of Phillips Laboratory

(Final Report for AFOSR Grant Number F49620-95-1-0285)

Bruce M. Boghosian, Principal Investigator
Center for Computational Science,
Boston University,
3 Cummington Street, Boston, Massachusetts 02215, U.S.A.

October 1, 1997

Abstract

This document is the final report for AFOSR Grant F49620-95-1-0285, "The Dynamics of Correlations in Lattice Gases." Under the terms of this grant, the Center for Computational Science at Boston University provided theoretical and computational support to the Lattice-Gas Theory and Computation group at the Geophysics Directorate of Phillips Laboratory (AFOSR task 2304CP). Twelve publications have resulted from this effort, as well as the sponsorship of the Sixth International Conference on Discrete Models for Fluid Mechanics, and the preparation of the proceedings of that meeting as a special issue of the *International Journal of Modern Physics C.* In addition to applying lattice-gas algorithms to systems of complex fluids and droplets, the work has resulted in two significant extensions of the lattice-gas algorithm: These are *integer lattice gases* which are proving to be an important methodology for the matching of microscopic, particulate, kinetic descriptions to macroscopic, continuum hydrodynamics, and *quantum lattice gases* which provide a paradigm for the simulation of physical systems on quantum computers. Moreover, we have shown that lattice-gas algorithms can be among the most efficient methods of simulating certain systems of interest in materials science, such as immiscible and amphiphilic fluids.

Contents

1 Historical Background

Hydrodynamic lattice-gas models were first proposed about ten years ago as an alternative strategy for computational fluid dynamics (CFD) [1, 2, 3]. Shortly after their introduction, it became clear that the methodology was capable of simulating fluids in situations for which conventional hydrodynamic models break down. For example, early studies showed how immiscible [4] and coexisting [5] phases could be simulated with simple lattice gas models. Previous studies of the breakdown of hydrodynamics in such situations had appealed to molecular dynamics (MD) simulations [6]. Gradually, lattice-gas methods began to find use as a computationally inexpensive alternative to MD. They provide a particulate model with an underlying kinetics which, though fictitious in its finest details, is capable of correctly treating many of the fundamental, universal properties of complex fluids, including multiphase coexistence, and droplet nucleation and growth.

The presence of an underlying particulate model can also be used to ensure the *stability* of the algorithm. Lattice gases based on an underlying particulate dynamics that obeys detailed balance have single-particle distribution functions that possess an H-theorem. From an algorithmic point of view, this feature prohibits high-wavenumber numerical instabilities of the sort that plagues many floating-point techniques. It was for these reasons that lattice-gas algorithms attracted the attention of members of the Geophysics Directorate of Phillips Laboratory who initiated AFOSR task 2304CP to study their application to droplet formation and other atmospheric phenomena.

Another historical development deserves to be mentioned in this context: In the late 1980's researchers working on lattice-gas theory derived the Boltzmann equation for the single-particle distribution function of LGA and realized that it could also be used as a viable simulation methodology in and of itself [7]. Since then, the Lattice Boltzmann (LB) method has grown in generality and has been simplified with the use of BGK collision operators [8]. Though it lacks the kinetic underpinnings and unconditional stability of LGA, it represents an important new family of physically motivated floating-point methods for simulating viscous fluid flow. In addition, two paradigms now exist for the LB treatment of complex-fluid hydrodynamics [9, 10]; indeed, one of these remains under active investigation in another ongoing study at Phillips Laboratory. The focus of this work, however, has been to find ways to take full advantage of the natural kinetic underpinnings and unconditional stability that LGA's have to offer. As will be described in later sections, some of our results may well offer new LB methods with improved stability properties, but we have not *assumed* LB algorithms at the outset of any of our studies. To make a rough analogy to the field of computational electronic structure, our methods bear the same relationship to LB methods as ab initio algorithms bear to Hartree-Fock methods.

Finally, another "spinoff" of lattice gases that shows great potential for the future is the method of Dissipative Particle Dynamics (DPD). The first papers on this method appeared in the early 1990's and were heavily influenced by the LGA methodology [11]. In particular, its developers wished to retain the advantage of a time step size comparable to the mean-free time, while allowing for a continuous and isotropic distribution of velocities, in order to avoid the many "lattice artifacts" that must be dealt with in LGA and LB simulations. Subsequent development of the method [12] has resulted in an algorithm that is very similar to MD, but allows for large time steps. The effects of the "fast" degrees of freedom that are ignored in this scenario are modelled by a combination of added dissipation and added noise, consistent with the fluctuation-dissipation theorem. These additions mitigate the problem of unlikely configurations that would otherwise arise from taking large time steps in an MD simulation, and effectively couple the microscopic dynamics to a heat bath. Like LGA, this method has been successfully applied to "accelerate" MD simulations of complex fluids [13]. Other methods considered for this purpose include Smoothed-Particle Hydrodynamics and the Generalized Consistent Boltzmann algorithm [14].

The escalation of interest in this field has led to a series of successful international meetings on "Discrete Methods of Fluid Mechanics." As part of the program of activity between Boston University and Phillips Laboratory, the sixth and most recent such meeting was sponsored at Boston University in August of 1996. The program of this meeting is presented in Appendix C. The proceedings of this meeting were published as a special issue of the *International Journal of Modern Physics C*; the table of contents of this special issue is presented in Appendix D. The preface to this proceedings acknowledged support of this grant [15].

2 Principal Areas of Study

2.1 Droplet Formation, Nucleation, Materials Science

Immiscible and coexisting fluid phases, as well as complex materials such as polymers, emulsions, colloids, glasses and granular materials, can exhibit emergent structure over a very wide range of length and time scales. Molecular dynamics (MD) simulations of such systems must evolve on femtosecond time scales, and are therefore not suitable for studying phenomena that develop on much longer mesoscopic and macroscopic time scales. The attraction of LGA for this area of study is that they offer a way to do a coarse-grained version of MD. In particular, because lattice-gas particles typically collide on the order of once per time step, they effectively allow for time steps sizes comparable to the mean-free time – roughly two orders of magnitude greater than what is possible with MD.

One area in which this has had great impact has been the study of droplets in microemulsions and amphiphilic fluids, and this has led to a productive collaboration with scientists at Schlumberger Research. In a 1996 paper in the *Proceedings of the Royal Society of London* [16], we showed how the lattice-gas methodology could be extended to model the mixture of two immiscible fluids plus a surfactant. Since surfactant particles have both hydrophyllic and hydrophobic regions covalently bonded together, they lower their free energy tremendously by residing on an interface. As a result, such fluids can require *extensive* amounts of interface in equilibrium. This requirement gives rise to the spontaneous self-assembly of stable droplets and/or extended structures. Depending upon the temperature, the extended structures can be either ordered (lyotropic, lamellar phases) or disordered (sponge phases). The characteristic sizes of the extended structures can be on the order of tens or hundreds of nanometers – much larger than a molecule, but much smaller than typical flow scales. This makes MD unsuitable for their efficient simulation, but it is often the only tool available, as hydrodynamic equations for these fluids are not known. This is then a perfect application for a *mesoscale* simulation technique, such as LGA.

In our first paper on this subject [16], we introduced a two-dimensional version of the LGA model, beginning with an existing immiscible lattice-gas model, and adding amphiphile particles with orientational degrees of freedom. The presence and orientation of the amphiphile particles contributed terms to the system Hamiltonian. To understand the nature of these, one should imagine that the primary immiscible phases are oppositely "charged," their tendency to separate owing to the predisposition of such opposite charges to repel. Pursuing this analogy, one can imagine that the surfactant particles are "dipole" particles in the very same sense. The terms in the system Hamiltonian have the effect of (i) causing the dipole particles to migrate to regions of strong order-parameter gradient, and to align with that gradient, and (ii) to interact with each other by dipole-dipole interactions. It is the first of these effects that gives rise to the tendency of the amphiphile to create interface; the second gives rise to a *curvature energy* of the surfaces thus formed.

Early in the study, we showed that the model had both a droplet phase and a sponge phase, depending only on the relative concentrations of water, oil and surfactant. These phases are illustrated in Figs. 1 and 2. The structure function corresponding to the order parameter was observed to evolve from a constant, corresponding to no structure at early times since the initial conditions were homogenized, to a peak that saturated at late times. The physical reason for the saturation is that further separation would result in too little interface to accomodate the amphiphile. The growth and saturation of the structure function is shown in Fig. 3.

The precise way in which the characteristic length scale

$$R(t) \sim \left(\frac{\int d^2k \; kS(k,t)}{\int d^2k \; S(k,t)} \right)^{-1}$$

saturates has been measured in experiments on the phase separation of block copolymers, and has been found to have the form of a stretched exponential,

$$R(t) \sim A - B \exp\left(-Ct^D\right).$$

Fig. 4 shows that we have found good agreement with this functional form, and we have also made predictions of the dependence of the coefficients C and D on the surfactant density [17].

Because equilibrium models of emulsion droplet and sponge phases have existed for about a decade, we made a conscious decision to focus our efforts on the study of nonequilibrium and hydrodynamic phenomena,

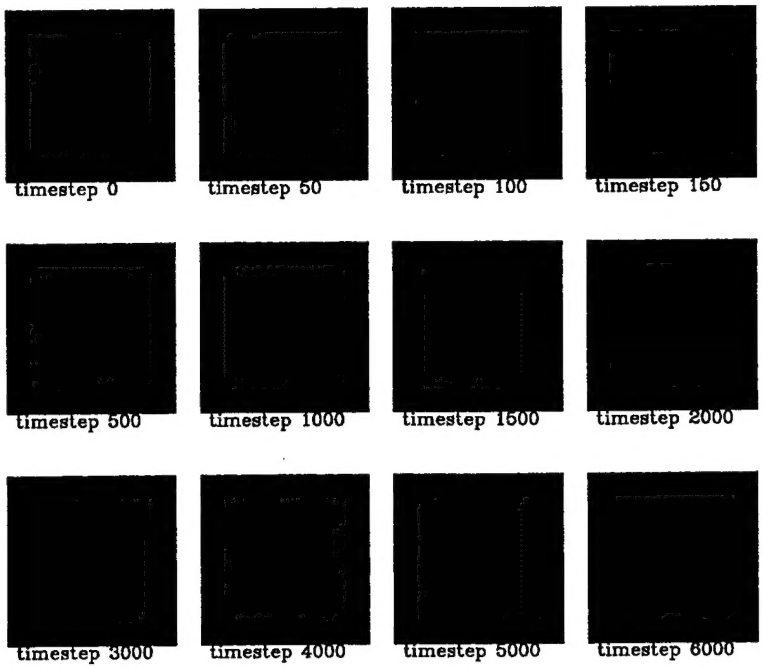

Figure 1: *Time evolution of droplet phase.*

Figure 2: *Time evolution of sponge phase.*

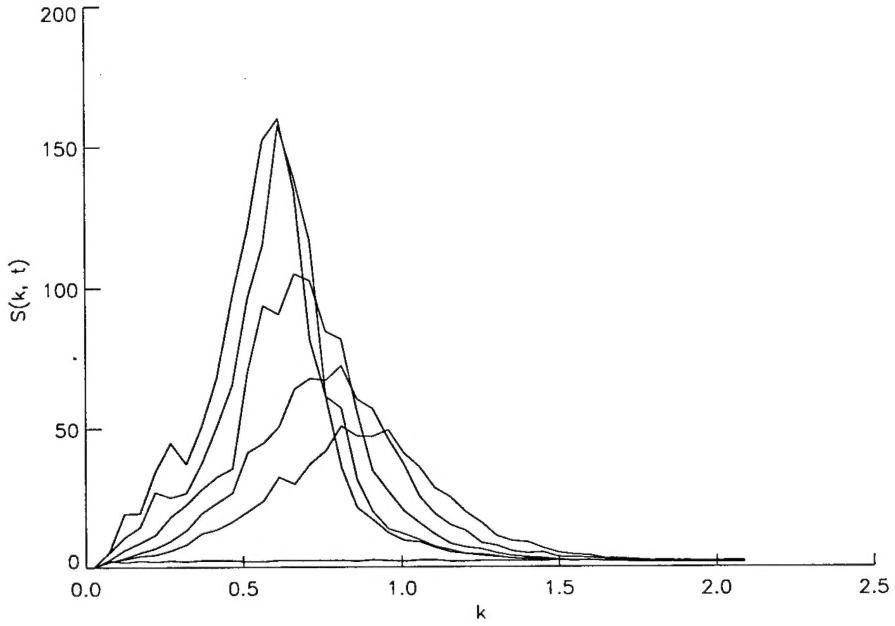

Figure 3: *Temporal evolution of $S(k,t)$ for microemulsion droplet case. Timesteps shown are, from bottom to top, $t = 0, 40, 80, 200, 800, 2000$.*

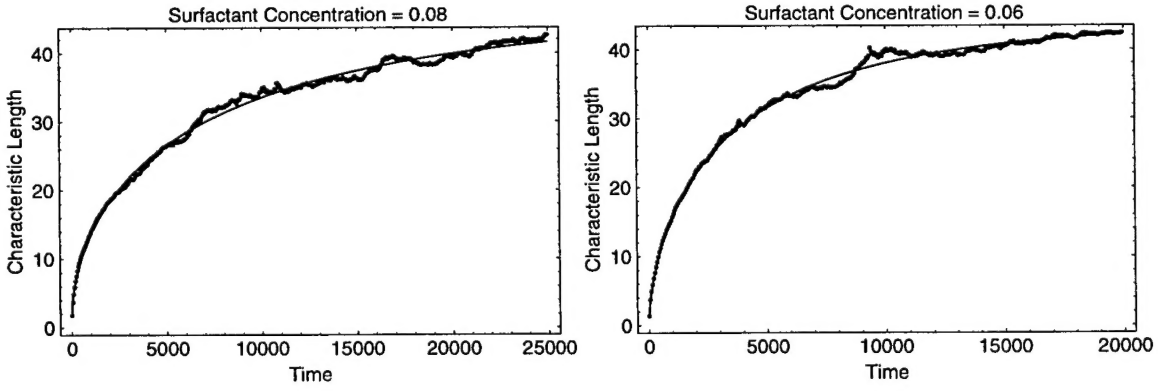

Figure 4: Fit of $R(t)$ to stretched exponential form for two different surfactant densities

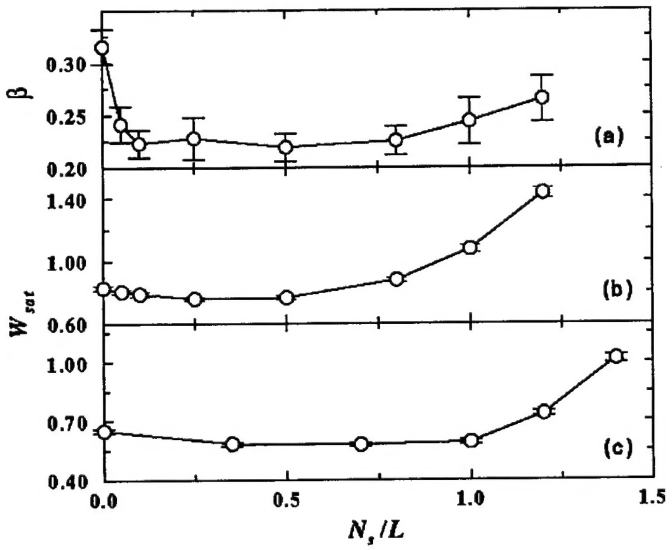

Figure 5: Plot of dynamic exponent β and saturated interfacial width against surfactant concentration

since those are areas for which our model is uniquely suited. Along these lines, in collaboration with Prof. H. Eugene Stanley and his group at Boston University, we studied the effect of surfactants on the interfacial fluctuations of such droplets. The results of this study were published in *Physical Review Letters* in 1996 [18]. Previous work [19] had shown that the dynamic exponents α and β governing the fluctuation of an interface between immiscible phases had the values 1/2 and 1/3, respectively. We showed that the presence of a small amount of surfactant changed both of these exponents significantly, but that in the dilute limit, for which the above-mentioned dipole-dipole interactions are unimportant, the quantity $\alpha(1+1/\beta)$ remained constant in the vicinity of 2. Moreover, we showed that the interfacial width could actually decrease to a minimum in the regime of dilute surfactant concentration; of course, further increase of surfactant concentration resulted in the widening and eventual destabilization of the interface. This is shown in Fig. 5. While a thorough theoretical explanation for this effect does not exist, our publication presents heuristic arguments in its support. Experimentalists at NIST have expressed great interest in this and related effects, and have encouraged us to pursue further simulations of it.

We have used the model to study two other phenomena that are known to experimentalists, but had been previously inaccessible to simulation. The first of these is the shear-induced sponge-to-lamellar phase transition. By modifying the boundary conditions to simulate oppositely moving boundaries, it is possible to create a shear flow. We then set the relative concentrations and Hamiltonian coupling coefficients to values that would yield a sponge phase in the absence of shear. Fig. 6 shows the time evolution of the same situation depicted in Fig. 2 in an imposed shear flow. The presence of the shear flow gives rise to lamellar structures clearly visible in the figure. This work was reported in detail in the *Journal of Physics, Condensed Matter* [20].

Another phenomenon that we have studied is the formation of so-called "multiemulsions" – possessing two distinct characteristic droplet sizes – in off-critical quenches from an initially homogenized state. Fig. 7, in which the two length scales are clearly visible, shows the time evolution of the multiemulsion. In a histogram of the droplet sizes, two peaks emerge; using this to define the two length scales, we plot their time development in Fig. 8. It is seen that the onset of the two length scales happens at finite time after the separation begins. This work has been published in *Physical Review E* [21].

Finally, we have exploited the fact that it is very straightforward to include chemical reactions in LGA models to simulate a well-studied experiment of Luisi [22]. The experiment was designed to study a simple protobiotic model of cell division. A mixture of oil and water is completely separated by a surface tension interface at the outset of the experiment. A chemical process is used to gradually convert a small amount of oil to an amphiphile. As the amphiphile builds up, it migrates to the interface where it eventually causes

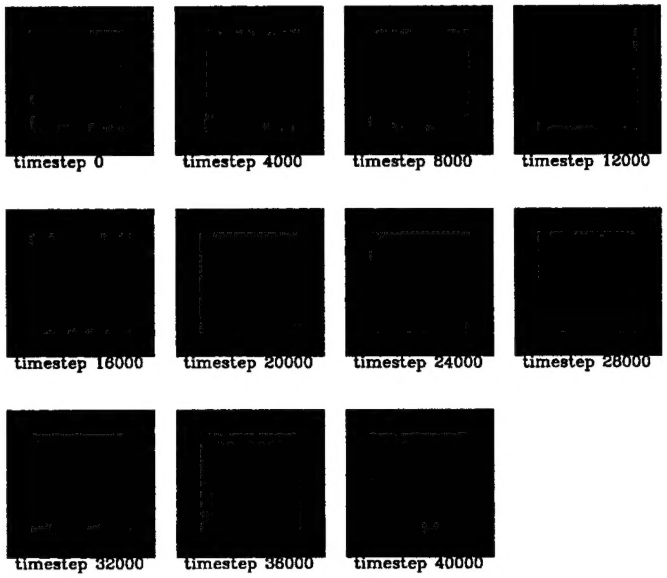

Figure 6: Shear-induced sponge-to-lamellar phase transition

Figure 7: Time development of multiemulsion

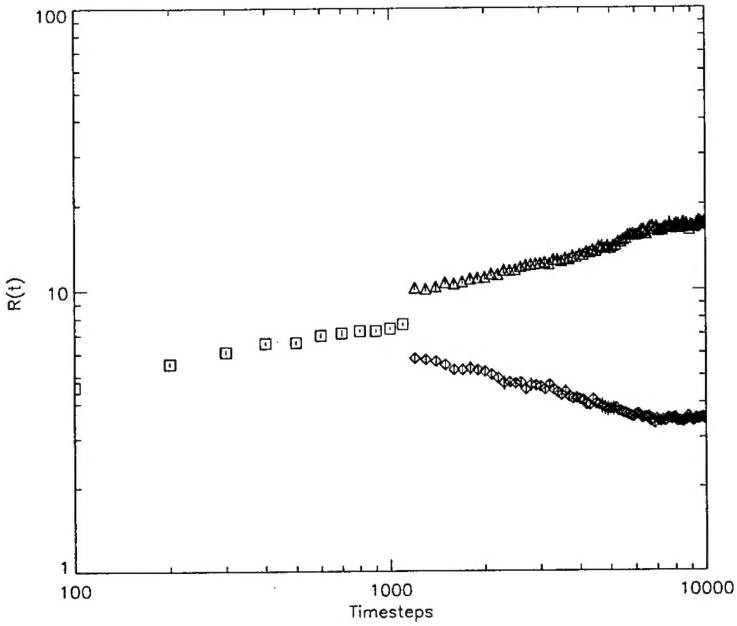

Figure 8: Time development of the length scales of the multiemulsion

spontaneous emulsification. The chemical process is such that micellized oil (that is, oil within emulsion droplets) has a higher probability of conversion to amphiphile than oil in bulk. The result is the formation of micellar "cells" which become unstable and divide with the buildup of amphiphile. This buildup is observed to be extremely rapid and consequently dependent to some extent on the underlying kinetics; bulk stochiometric rate equations are utterly unable to predict the time development, though modified theoretical treatments [23] using Becker-Doering nucleation theory have captured the essential physical mechanisms. Both Luisi's experimental data for the buildup of micelles and our simulation results are shown in Fig. 9. Our paper describing these results was published in the *Journal of the American Chemical Society* [24].

2.2 Integer Lattice Gases

Since studies of both LGA and LB take place at Phillips Laboratory, there is naturally a great deal of interest in comparing the two techniques, and in understanding their relative advantages and disadvantages. As noted in Section 1, the very first LB methods had their origin in studies of the Boltzmann equation of LGA [7]. Subsequent studies replaced the LGA collision operators with simplified, BGK collision operators [8]. Lacking a particulate foundation and any analog of a detailed-balance condition, the argument can be made that lattice Boltzmann algorithms are really nothing more (or less) than an entirely new class of explicit finite-difference methods. As such, it is only to be expected that they share some of the advantages and disadvantages inherent to finite-difference schemes. One important advantage is that they involve continuum-valued quantities, and are therefore very amenable to computer implementation using floating-point arithmetic. A disadvantage is that they are subject to numerical instability. Indeed, such instabilities have been observed in lattice Boltzmann treatments of the Navier-Stokes equations, and the precise conditions for their onset are poorly understood at present.

Hydrodynamic LGA models that lack numerical instabilities have been known for over a decade. It is worthwhile to spend a moment examining the underlying reason why such models exist. Of course, LGA are based on an underlying particulate dynamics that conserves mass and momentum exactly, and it is tempting to think that this is how they manage to avoid numerical instability, but such is not the case. It has been shown [25] that certain LGA with exactly conserved mass and momentum are subject to bizarre numerical instabilities in which, for example, the anisotropy of the underlying lattice may make itself manifest. So

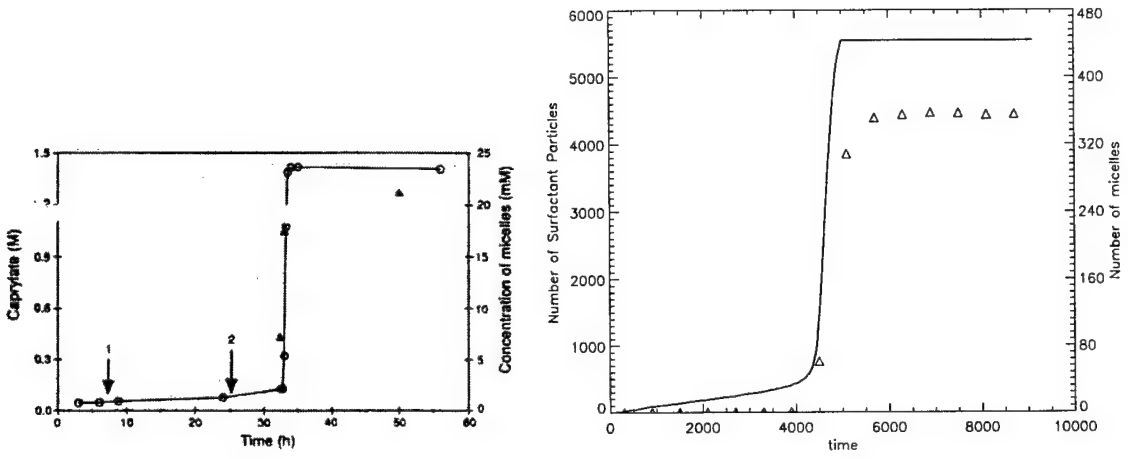

Figure 9: Comparison of experimental results for micelle buildup (left) to simulation results (right)

exact conservation does not ensure numerical stability.

The property that *is* shared by all known numerically stable and thermodynamically consistent LGA models is that their underlying particulate dynamics obeys the condition of *detailed balance* (DB). This condition is a probabilistic version of microscopic reversibility. For a system that may make transitions from a state s to a new state s', DB requires that the associated transition probability $A(s \to s')$ obey the equation

$$P(s)A(s \to s') = P(s')A(s' \to s),$$

where $P(s)$ is the probability that the system is in a state s. DB is a sufficient condition for the derivation of an H-theorem in LGA models. The H-theorem provides a Lyapunov function that decreases monotonically until it reaches a minimum which corresponds to thermodynamic equilibrium. The existence of the Lyapunov function thus ensures the stability of the equilibrium state. For systems sufficiently near equilibrium – for example, hydrodynamic systems for which the approximation of *local thermodynamic equilibrium* is a good one – the growth of a numerical instability would be in gross contradiction to the monotonicity of H. So DB is the principal property precluding numerical instability.

It would therefore be most useful to find some kind of model intermediate to the LGA and LB levels of description. Most ideal would be a model that could be implemented using floating-point arithmetic, but which still retained enough of a particulate basis to obey a DB condition. To the extent that LGA methods are based on the manipulation of bits, and LB methods are based on that of floating-point numbers, one is tempted to search for LGA models based on integers. We have done this, and have published a paper on our work in *Physical Review E* in 1996 [26]. Our work is ongoing, however, and we expect to produce at least one further paper on the subject soon.

We found that the ability to have more than a single particle moving along each lattice vector allowed us to fix numerous well known pathologies of LGA. For example, since a lattice constitutes a preferred galilean frame of reference, LGA are subject to violations of galilean invariance that can survive the hydrodynamic limit. Such violations give rise to a spurious factor, denoted by g, multiplying the convective term of the emergent Navier-Stokes equation. We found that this factor depends critically on the maximum number of particles per direction. In particular, if the average number of particles per direction is much smaller than the maximum number of particles per direction, the g factor goes to unity, so there is no problem.

In our paper on this subject, we considered lattice gases with L bits of information per lattice vector that were binary encoded to represent from 0 to $2^L - 1$ particles per lattice vector. For lattice gases with n lattice vectors and n_r rest particles per site on a D dimensional Bravais lattice, we found that galilean invariance ($g = 1$) was recovered when

$$G_L = \left(1 + \frac{2}{D}\right)\left(\frac{n}{n + n_r}\right),$$

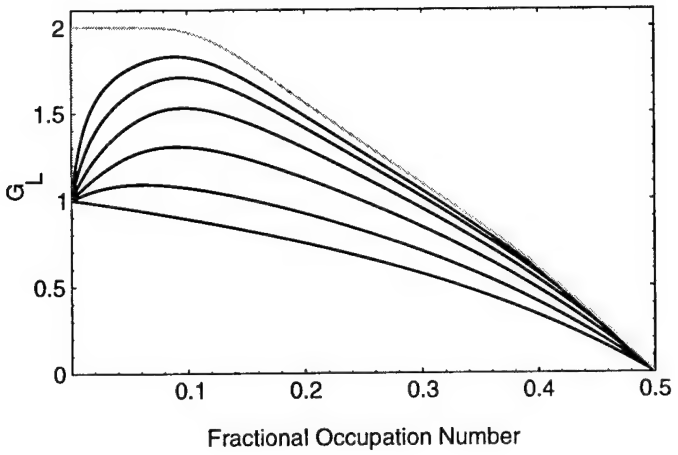

Figure 10: G_L versus f for several values of L. The black curves represent L values from 1 to 6, increasing upward, while the gray curve is the limit as $L \to \infty$.

where G_L is plotted as a function of the fractional occupation number f in Fig. 10. We see that for each value of L there are certain critical filling fractions f for which Galilean invariance is recovered. These critical values of f are tabulated in Fig. 11. Since the publication of this paper, we have developed more sophisticated methods of attaining $g = 1$ that are valid over a wider range of densities.

Another motivation of the integer LGA approach is the desire to control the level of the statistical noise that is inherent to LGA models. Since a channel of L bits can carry up to $2^L - 1$ particles, one might hope that the noise would reduce by a factor of the inverse square root of that – something like $2^{-L/2}$. Unfortunately, this does not turn out to be the case. The noise does reduce, but only algebraically in L. The detailed reason is given in the published paper; here we plot the noise level versus the fractional occupation number for several different values of L in Fig. 12 to demonstrate the decrease that does result. Once again, since the publication of this paper, we have developed more sophisticated ways of reducing the noise; these will be published in the near future.

Our level of interest in integer LGA remains high for two reasons. The first is that investigations along these lines may give rise to unconditionally stable LB algorithms. The second has to do with one of the current frontiers of computational physics research – namely, the exploration of so-called *multiscale* or *multiphysics* algorithms. These are algorithms where different physical models are used in an adaptive fashion. They are the next level of algorithmic sophistication beyond Adaptive Mesh Refinement (AMR) algorithms. In AMR algorithms, one changes the refinement of the grid adaptively; in multiphysics algorithms, one actually changes the physical model being used in an adaptive fashion. One particular area of interest, for example, is the "matching" of MD to hydrodynamics. One would like to be able to treat situations for which certain portions of the domain must be described at the kinetic level, while others can be described at the hydrodynamic level. An integer LGA would seem to provide an ideal way to treat this situation: Particles represented by integers, moving about on one portion of the grid, could merge smoothly with hydrodynamic quantities represented by real numbers and obeying a LB equation in other portions.

2.3 Quantum Lattice Gases

Finally, over the past two years, there has been a growing interest in Quantum Lattice-Gas Automata (QLGA). To the extent that the LGA and LB methods can be thought of as discrete bits and real-valued quantities moving about on a grid, respectively, then a QLGA for a single quantum particle can be thought of as complex amplitudes doing likewise and colliding according to unitary transformations at each site. Just as the real-valued quantities of the LB method represent occupation probabilities, so do the squares of the moduli of the complex amplitudes of a QLGA. As these amplitudes move about and collide on the spatial grid, they can *interfere* with each other, giving rise to behavior that is not possible with ordinary lattice gas

FHP Lattice Gas ($D = 2$, $n = 6$)			
n_r	L	Low-Density Root	High-Density Root
0	∞	0.0	0.0
1	6	0.0396831	0.143848
	∞	0.0	0.168451
2	4	0.0704358	0.126560
	5	0.0322583	0.177356
	6	0.0158730	0.195949
	∞	0.0	0.212636
4	3	0.0362392	0.167555
	4	0.0166667	0.228582
	5	0.0080645	0.253770
	6	0.0039683	0.265426
	∞	0.0	0.276535

FCHC Lattice Gas ($D = 4$, $n = 24$)			
n_r	L	Low-Density Root	High-Density Root
0	4	0.0704358	0.126560
	5	0.0322583	0.177356
	6	0.0158730	0.195949
	∞	0.0	0.212636
1	4	0.0528917	0.152419
	5	0.0253456	0.193030
	6	0.0124717	0.209795
	∞	0.0	0.225163
2	4	0.0417410	0.171769
	5	0.0201613	0.207212
	6	0.0099206	0.222576
	∞	0.0	0.236849
4	3	0.0654937	0.120009
	4	0.0266677	0.203001
	5	0.0129032	0.232239
	6	0.0063492	0.245488
	∞	0.0	0.257994

Figure 11: Values of $f \in (0, 1/2)$ such that $g = 1$

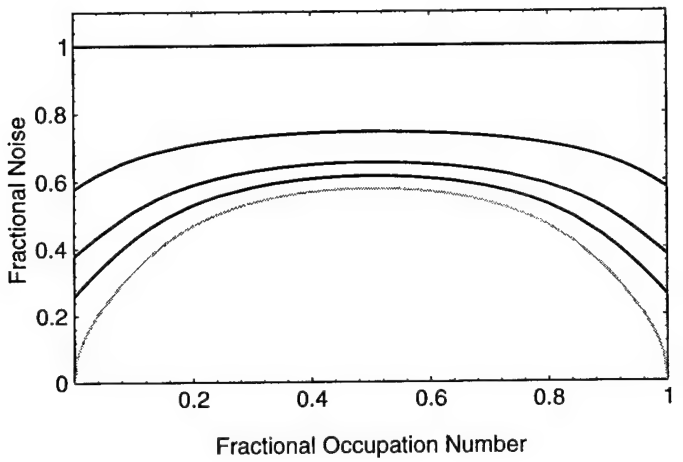

Figure 12: $\Delta\mathcal{F}_L$ versus f for several values of L. The black curves represent L values from 1 to 4, increasing downward, while the gray curve is the limit as $L \to \infty$.

automata.

Whereas an LGA with N bits can be in any one of 2^N distinct states, a QLGA can be in a complex superposition of *all* of those 2^N states – although conservation of mass (and momentum if appropriate) restricts the evolution to particular sectors of the full Hilbert space. It follows that in order to consider QLGA with more than a single particle, it is necessary to add dimensions to the configuration space for each additional particle. This becomes rapidly intractable on any classical computer, but is easily seen to pose no extra problem for a quantum computer [27, 28]. Indeed, QLGA can be regarded as a novel paradigm for computational physics on quantum computers.

We have shown that the generic behavior of a quantum lattice gas with scattering matrices at each site that are both unitary and invariant under the (Cartesian) lattice rotation group is that of Schrödinger's equation. To get an idea of why this should be the case, consider a lattice-Boltzmann model with configuration space defined by two complex fields, $\psi_1(x,t)$ and $\psi_2(x,t)$, taking independent values on a lattice with one spatial dimension x and one temporal dimension t. Define the dynamics of this model to obey the equations

$$\psi_1(x+1,t) = \frac{1}{2}\left[(1-i)\psi_1(x,t-1) - (1+i)\psi_2(x,t-1)\right]$$

$$\psi_2(x-1,t) = \frac{1}{2}\left[(1-i)\psi_2(x,t-1) - (1+i)\psi_1(x,t-1)\right].$$

These equations give a unitary time evolution to ψ. To understand how ψ evolves in a continuum limit, we can expand the equations of motion through 4 time steps, giving for example

$$\begin{aligned}\psi_1(x,t+4) &= \frac{1}{4}\left[-\psi_1(x-4,t) + 3\psi_1(x-2,t) + \psi_1(x,t) + \psi_1(x+2,t)\right] \\ &\quad + \frac{i}{4}\left[\psi_2(x-2,t) - \psi_2(x,t) - \psi_2(x+2,t) + \psi_2(x+4,t)\right].\end{aligned}$$

Taking a continuous limit as the lattice spacing scales as ϵ in the x direction and ϵ^2 in the t direction, we find the differential equation

$$\partial_t \psi_1(t) = \frac{i}{2}\partial_x^2 \psi_2(t)$$

A similar equation holds for ψ_2, and so it follows that

$$\partial_t(\psi_1 + \psi_2) = \frac{i}{2}\partial_x^2(\psi_1 + \psi_2).$$

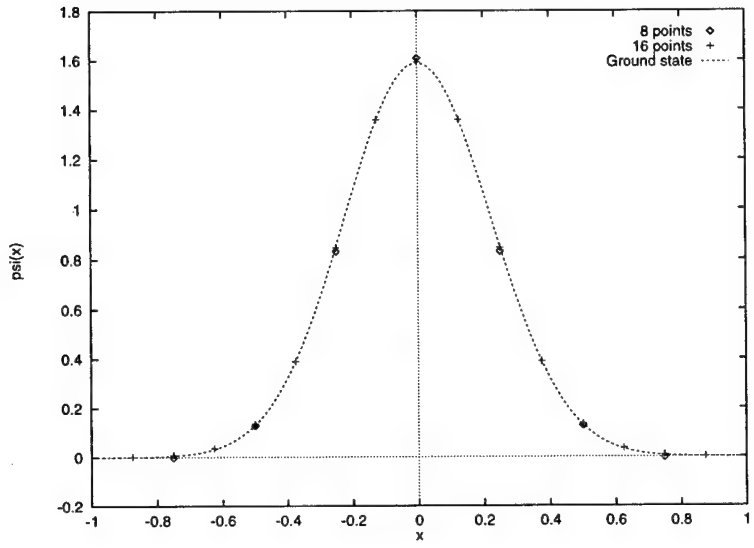

Figure 13: Ground state in quadratic potential with 8 and 16 lattice sites

Thus, we see that the total amplitude $\Psi(x,t) = \psi_1(x,t) + \psi_2(x,t)$ satisfies a Schrödinger equation. Our papers on this subject go into much more detail, extending the above treatment to the case of many quantum particles, and to Hamiltonians that include both applied and interparticle potentials. Figs. 13 and 14 show QLGA simulations of a single particle in a harmonic oscillator potential.

The emergence of Schrödinger's equation in this context is fascinating for several reasons: First, it shows that Schrödinger evolution is the *emergent* behavior of a wide class of discrete microscopic dynamical systems. Second, since QLGA bear the same relationship to LGA that quantum computation bears to classical computation, this observation effectively provides an entirely new paradigm for quantum computation; indeed, it provides a method of simulating arbitrary quantum mechanical systems on a quantum computer in a time that scales polynomially with the number of quantum particles in the system. Third, even on the ordinary "classical" computers of today, it yields a completely new and unexpected fully explicit finite-difference algorithm for Schrödinger's equation. Fourth, because there is a simple nonlinear transformation relating Schrödinger's equation and Euler's equation for an inviscid fluid, it provides us with a new method to simulate fully compressible (albeit irrotational) Euler flow on a Cartesian lattice.

It is worth expanding upon the second point made above. Let us consider a system of n particles moving on a D-dimensional lattice of size $l = q^D$, with $m = 2D$ allowed particle positions per lattice site (Cartesian lattice). Assuming that $n \ll lm$, the number of complex variables needed to describe the state of the system at a point in time is

$$\frac{(lm)!}{n!(lm-n)!} \sim \frac{(lm)^n}{n!}. \tag{1}$$

To simulate a system with this number of variables on a classical computer would take at the very least on the order of the number of variables for each time step. The number of time steps needed scales as q^2 (because t scales as ϵ^2), so the total time needed for a computation on a classical computer would be

$$T_c \approx \mathcal{O}(\frac{q^{2+Dn} m^n}{n!}) \tag{2}$$

For a typical calculation of physical interest, we might have $n = 100, q = 20, D = 3$. For such a calculation, the number of operations needed on a classical computer would be on the order of $T_c \approx 10^{312}$. This is clearly impractical. Note that a standard finite difference method would eliminate the factor of m^n in (2), however this would not make such a calculation any more accessible. Only when the number of particles n is extremely small is it conceivable that these algorithms might be a useful approach for simulating quantum systems on a classical computer.

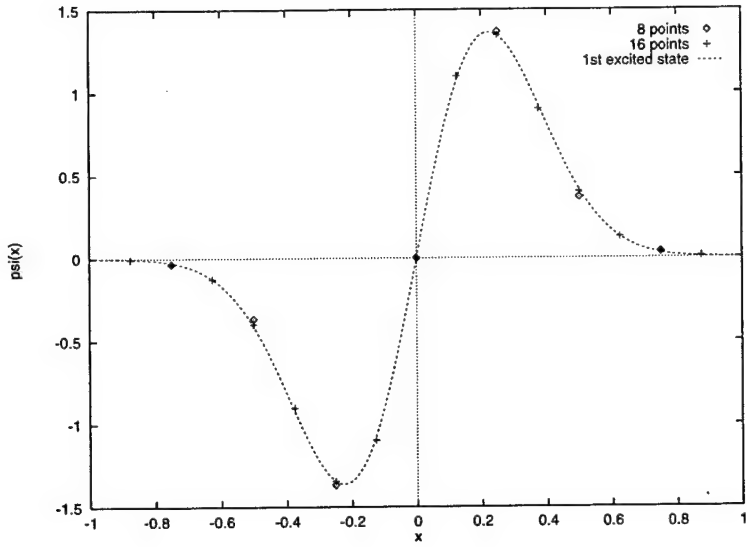

Figure 14: First excited state in quadratic potential with 8 and 16 lattice sites

Now let us consider the computational complexity of the same algorithms on a quantum computer. For the quantum simulation, we need $m \cdot l$ quantum bits (sometimes called "qubits"). The local advection and collision steps can be accomplished with on the order of $m \cdot l$ quantum operations per time step. Thus, a system of quantum particles which affect one another only through local interactions can be simulated on a quantum computer in time on the order of

$$T_q \approx \mathcal{O}(2Dq^{2+D}). \tag{3}$$

Note that this time is *independent* of the number of particles n being simulated. In fact, this algorithm will simultaneously simulate the system for all allowed numbers of particles $n \leq lm$ in the same time it takes to simulate a system with only a single particle. With the numbers used in the example above on a classical machine, the number of operations needed to perform the simulation is a much more tractable $T_q \approx 19.2 \cdot 10^6$. The idea that it might be possible to simulate quantum mechanical systems exponentially faster on a quantum computer than on a classical computer was first suggested by Feynman[29]; a general argument for this conclusion was given more recently by Lloyd[30]. The algorithms that we have developed represent a concrete instantiation of the general principles discussed by those authors.

We have published three papers on our work in this area – the first is about to appear in *Physical Review E* [28], the second is pending in the *International Journal of Modern Physics C* [31], and the third has appeared in the *Proceedings of PhysComp '96* [32]; the last of these is the proceedings of an international meeting on physical computation that was held at Boston University last year. Also, Jeffrey Yepez of Phillips Laboratory has used this approach directly to develop a new lattice-gas model of Helium II. His idea was to couple a quantum lattice gas for the superfluid, which obeys Schrödinger's equation, and a classical lattice gas for the normal fluid which has nonzero viscosity, dissipation, etc.

3 Conclusions

We have described the program of activity of the lattice-gas research collaboration between the Boston University Center for Computational Science and the Geophysics Directorate of Phillips Laboratory (under AFOSR task 2304CP). This collaboration has centered on three major areas of study: (i) droplet formation and materials science, (ii) integer lattice gas automata, and (iii) quantum lattice gas automata. Area (i) is the application of lattice-gas methodologies to complex hydrodynamic phenomena, while areas (ii) and (iii) are substantial extensions of the lattice-gas paradigm. We have provided a detailed account of the

principal new results in all three of these areas. Twelve publications have resulted from this effort, as well as the sponsorship of the Sixth International Conference on Discrete Models for Fluid Mechanics, and the preparation of the proceedings of that meeting as a special issue of the *International Journal of Modern Physics C*.

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A Publications

The following twelve publications acknowledged the support of this grant:

1. Weig, F.W.J., Coveney, P.V. Coveney, B.M. Boghosian, "Lattice-Gas Simulations of Minority-Phase Domain Growth in Binary Immiscible and Ternary Amphiphilic Fluid," *Physical Review E* (to appear, 1997).

2. A.N. Emerton, P.V. Coveney, B.M. Boghosian, "Shear Induced Isotropic-to-Lamellar Transition in a Lattice-Gas Automaton Model of Microemulsions," *J. Phys.: Cond. Mat.* (to appear, 1997).

3. A.L. Garcia, F.J. Alexander, B.J. Alder, "A Particle Method with Adjustable Transport Properties – The Generalized Consistent Boltzmann Algorithm," *J. Stat. Phys.*, (to appear, 1997).

4. B.M. Boghosian, F.J. Alexander, P.V. Coveney, "Discrete Models of Complex Fluid Dynamics," preface for the Proceedings of the Sixth International Conference on Discrete Fluid Mechanics, *International Journal of Modern Physics C* (August, 1997).

5. B.M. Boghosian, W. Taylor, "Quantum Lattice-Gas Models for the Many-Body Schrodinger Equation," preprint BU-CCS-970102, PUPT-1677, prepared for the Proceedings of the Sixth International Conference on Discrete Fluid Mechanics, *International Journal of Modern Physics C* (August, 1997).

6. B.M. Boghosian, W., Taylor, "Quantum Mechanics on a Quantum Computer," preprint BU-CCS-960603, *Proceedings of PhysComp '96* (to appear, 1997).

7. F.W. Starr, S.T. Harrington, B.M. Boghosian, H.E. Stanley, "Interface Roughening in a Hydrodynamic Lattice-Gas Model with Surfactant," *Phys. Rev. Lett.* **77** (14 October, 1996) 3363-3366.

8. B.M. Boghosian and W. Taylor, "A Quantum Lattice-Gas Model for the Many-Particle Schrödinger Equation in d Dimensions," *Physical Review E* (August, 1997).

9. A.N. Emerton, P.V. Coveney, B.M. Boghosian, "Domain Growth in Immiscible Fluids and Microemulsions," *Physical Review E*, **55** (January, 1997) 708-720.

10. P.V. Coveney, A.N. Emerton, B.M. Boghosian, "Simulation of Self-Reproducing Micelles Using a Lattice-Gas Automaton," *Journal of the American Chemical Society* **118** (1996) 10719-10724.

11. B.M. Boghosian, J. Yepez, F.J. Alexander, N.H. Margolus, "Integer Lattice Gases," *Physical Review E* **55** (April, 1997) 4137-4147.

12. B.M. Boghosian, P.V. Coveney, A.N. Emerton, "A Lattice-Gas Model of Microemulsions," *Proc. Roy. Soc A* **452** (8 May, 1996) 1221-1250.

B Invited Talks and Presentations

The following invited talks and presentations were related to the topic of this grant proposal, and were presented during the time period of the grant or immediately thereafter:

1. Plenary speaker, Physics Computing '97, American Physical Society, Santa Cruz, California (August, 1997).
2. Course speaker, Department of Materials Science, Massachusetts Institute of Technology, Cambridge, Massachusetts (18 April, 1997).
3. Colloquium speaker, Department of Physics, University of Pittsburgh, Pittsburgh, Pennsylvania (10 April, 1997).
4. Seminar speaker, Department of Physics, University of Massachusetts, Amherst, Massachusetts (November, 1996).
5. Seminar speaker, Center for Interdisciplinary Research on Complex Systems, Northeastern University (May 7, 1996).
6. Session organizer, Monte Carlo Methods in Computational Physics, American Physical Society Annual Meeting, Indianapolis, Indiana (May 2-5, 1996).
7. Colloquium speaker, Department of Mechanical Engineering, Massachusetts Institute of Technology (April, 1996).
8. Session speaker, American Physical Society Topical Meeting on Condensed Matter, St. Louis, Missouri (March 21, 1996).
9. IAP Seminar on Molecular Modelling, Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts (January 29, 1996).
10. 74th Statistical Physics Conference, Hill Center, Rutgers University, Piscataway, New Jersey (Dec. 17-19, 1995).
11. Nanotechnology Forum, Laboratory for Computer Science, Massachusetts Institute of Technology (December 5, 1995).
12. Colloquium speaker, Department of Physics, Boston University, Boston, Massachusetts (October 31, 1995).
13. Nonlinear Optics Workshop, University of Arizona, Tucson, Arizona (October 1-3, 1995).
14. Lattice Gas Automata Workshop, National Institute of Standards and Technology, Gaithersburg, Maryland (August 22, 1995).
15. Seminar speaker, Department of Applied Science, University of California, Davis/Livermore, Livermore, California (May 16, 1995).
16. Seminar speaker, Department of Mechanical Engineering, Massachusetts Institute of Technology (May 8, 1995).
17. Seminar speaker, Center for Computational Science, Boston University, Boston, Massachusetts (March 17, 1995).
18. S.I.A.M. Seminar on Parallel Scientific Computation, San Francisco, California (February 17, 1995).
19. Seminar speaker, Institute for Scientific Computing, Lawrence Livermore National Laboratory, Livermore, California (February 13, 1995).
20. I.A.P. Seminar on Molecular Modelling, Department of Nuclear Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts (January 25, 1995).

21. Seminar speaker, I.B.M., T.J. Watson Research Center, Yorktown Heights, New York (November 10, 1994).

22. Seminar speaker, Center for Computational Science, Boston University, Boston, Massachusetts (October 7, 1994).

23. Colloquium speaker, Physics Department, Clark University (September 22, 1994).

C Sixth International Conference on Discrete Models for Fluid Mechanics

Boston University Center for Computational Science, Boston, Massachusetts, USA

August 26-28, 1996

Monday, August 26, 1996

The following is the complete agenda for the Sixth International Conference on Discrete Models for Fluid Mechanics, held at the Metcalf Science Center at Boston University on 26-28 August 1996. The proceedings of the conference were published as a special issue of the *International Journal of Modern Physics C* (Vol. 8, No. 4, August, 1997). The table of contents of this issue is presented in the following appendix.

C.1 Invited and Contributed Talks

08:00 - 08:20 Registration and Coffee

08:20 - 08:30 Bruce Boghosian (Boston University) Welcoming Remarks

08:30 - 08:40 Roscoe Giles (Boston University Deputy Director, Center for Computational Science) Welcoming Remarks

Session I: Lattice Models I *Chair: Peter Coveney*

08:40 - 09:10 Hudong Chen (Exa Corporation) "Digital Physics: Basic Concept and Some Applications"

09:10 - 09:40 Gary Doolen (LANL) "Applications for which the Lattice Boltzmann Method Works Best"

09:40 - 09:55 Xiaoyi He (LANL) "Discretization of the Continuous Boltzmann BGK Equation and its Applications"

09:55 - 10:10 Nicolas G Hadjiconstantinou (MIT) "Heterogeneous Atomistic–Continuum Methods for Dense Fluid Systems"

10:10 - 10:30 Posters, Coffee

Session II: Multiphase Flow I *Chair: Gary Doolen*

10:30 - 11:00 Peter Coveney (Schlumberger Cambridge Research) "Lattice Gas Automaton Models of Amphiphilic Systems"

11:00 - 11:30 Shi Jin (Georgia Institute of Technology) "Kinetic Relaxation Schemes for Compressible Hydrodynamics"

11:30 - 12:00 Jean-Pierre Boon (Brussels) "Entropy and correlations in lattice gas automata without detailed balance"

12:00 - 12:15 Joel Mozer (Phillips Laboratory) "A new approach to radiative transfer through clouds using the lattice-Boltzmann method"

12:15 - 13:30 Lunch

Session III: Lattice Models of Single-Phase Fluids *Chair: Jean-Pierre Boon*

13:30 - 14:00 Laurent Giraud (C.N.R.S.) "A Lattice Boltzmann Model for Visco-elastic Fluids"

14:00 - 14:30 Kun Xu (Princeton University) "BGK-based Schemes for the Simulation of Compressible Flow"

14:30 - 15:00 Shiyi Chen (IBM, Watson) "Finite Difference Lattice Boltzmann Equation and Boundary Conditions"

15:00 - 15:20 Posters, Coffee

Session IV: Particulate Models I *Chair: Shiyi Chen*

15:20 - 15:50 Jayanth Banavar (Pennsylvania State University) "Continuum Deductions from Molecular Hydrodynamics"

15:50 - 16:20 Turab Lookman (U.W. Ontario) "Mesoscopic hydrodynamics with BGK methods"

16:20 - 16:50 Lukas Wagner (Ohio State University) "Molecular Dynamics Simulation of Spreading Droplet Dynamics"

16:50 - 17:20 Pep Espanol (Madrid) "Dissipative Particle Dynamics and Fluid Particle Dynamics"

Tuesday, August 27, 1996

Session V: Lattice Models II *Chair: Frank Alexander*

08:25 - 08:55 Yu Chen (U. Tokyo) "Several improvements on the lattice BGK simulation of fluid flow"
08:55 - 09:25 Norman Margolus (Boston University) "Crystalline Computation"
09:25 - 09:55 Li-Shi Luo (LANL) "Some New Developments of the Lattice Boltzmann Method"
09:55 - 10:10 Alberto Suarez (Brussels) "Fluctuations in Diffusive Lattice Gas Automata"
10:10 - 10:30 Posters, Coffee

Session VI: Multiphase Flow II *Chair: Jeff Yepez*

10:30 - 11:00 Xiaowen Shan (Los Alamos National Laboratory) "Lattice-Boltzmann Methods for Modelling Complex Fluids"
11:00 - 11:30 Julia Yeomans (Oxford University) "Lattice Boltzmann Simulations of Multiphase Fluids"
11:30 - 12:00 Yasuyoshi Kato "AMADEUS Project and Microscopic Simulation of Boiling Water Two-Phase Flow by Lattice Boltzmann Method"
12:00 - 13:30 Lunch

Session VII: Interfaces, Rheology *Chair: Sauro Succi*

13:30 - 14:00 Anthony Ladd (LLNL) "Deformation and failure in microstructural materials"
14:00 - 14:30 Eirik Flekkoy (Oslo) "Fluctuating Hydrodynamic Interfaces: Theory and Lattice Gas Simulation"
14:30 - 15:00 Ali Nadim (Boston University) "Constitutive Equations for Dilute Emulsions of Viscous Drops with Interfacial Rheology"
15:00 - 15:15 Yasuhiro Hashimoto (The University of Tokyo) "Measurement of Ascending Velocity and Surface Transformation of a Drop Using the Lattice Gas Method"
15:15 - 15:30 Francis Starr (Boston University) "Interface Roughening in a Hydrodynamic Lattice-Gas Model with Surfactant"
15:30 - 15:50 Posters, Coffee

Session VIII: Chemical Reactions, Combustion, and Other Applications *Chair: Tony Ladd*

15:50 - 16:20 Ray Kapral (University of Toronto) "Front Bifurcations, Phase Transitions and Knots in Bistable Reacting Systems"
16:20 - 16:50 Yue-Hong Qian (Columbia) "Behavior near the Critical Point in Liquid-Gas Phase Transitions"
16:50 - 17:05 Steen Rasmussen (LANL) "Lattice Gasses, Molecular Self-Assembly, and Dynamical Hierarchies"
17:05 - 17:35 Sauro Succi (Istituto Applicazioni Calcolo, Rome) "New applications of old lattice Boltzmann schemes: numerical combustion"
17:35 - 17:50 Neil Simons (Ottawa) "Application of Lattice Gas Automata to the Solution of Electromagnetic Field Problems"
18:30 **Banquet**
Panel Discussion: *Moderator* Matthieu Ernst
Participants Julia Yeomans, Dan Rothman, Ray Kapral, Xiaowen Shan, Antoine Schlijper, Pep Espanol

Wednesday, August 28, 1996

Session IX: New Vistas in Theory and Simulation *Chair: Norman Margolus*

08:10 - 08:40 David Meyer (UCSD) "Quantum Lattice Gases"
08:40 - 09:10 Washington Taylor (Princeton University) "Quantum Lattice Gas Models of Nonrelativistic Many-Body Quantum Mechanics"
09:10 - 09:40 Brosl Hasslacher (LANL) (TBA)
09:40 - 10:10 Jeffrey Yepez (Phillips Laboratory) "Lattice-Gas Methods for Modelling Complex Fluids"
10:10 - 10:30 Posters, Coffee

Session X: Porous Media *Chair: Wati Taylor*

10:30 - 11:00 John Olson (MIT) "Lattice Gas Simulations of Two-Fluid Flow in Sedimentary Rock"

11:00 - 11:15 Manuel Schulz (University of Dortmund) "Simulation and Visualization of transient 3D-Flow in arteries with an artificial heart valve using Lattice-Boltzmann Methods"

11:15 - 11:45 Olav van Genabeek (MIT) "Statistics of Slow Flow Through Complex Structure"

11:45 - 12:15 Nicos Martys (NIST) "Single and Multicomponent flow in Porous Media"

12:15 - 12:30 Ruud van der Sman (Agrotechnological Research Institute, Netherlands) "Lattice Boltzmann scheme for Natural Convection in Porous Media"

12:30 - 14:00 Lunch

Session XI: Particulate Models II *Chair: John Olson*

14:00 - 14:30 Francis J. Alexander (Boston University) "The Direct Simulation Monte Carlo Method: New Directions"

14:30 - 15:00 Christopher Lowe (FOM, Amsterdam) "Simulating the effect of fluid flow on aggregation"

15:00 - 15:20 Posters, Coffee

Session XII: Particulate Models III *Chair: Bruce Boghosian*

15:20 - 15:50 Matthieu Ernst (Utrecht) "Dissipative Particle Dynamics, in Models for Granular Materials: Both Simulations, Microscopic Theory and Linear and Nonlinear Stability Theory"

15:50 - 16:20 Antoine Schlijper (Shell Laboratories, Amsterdam) "Modelling of Polymer Solution Rheology by Dissipative Particle Dynamics"

16:20 - 16:35 Keir Novik (Cavendish Laboratory) "Domain growth and phase separation in binary immiscible fluids using dissipative particle dynamics"

16:35 - 17:05 Charles Wingate (LANL) "Smooth Particle Hydrodynamics"

17:05 - 17:15 Claudio Rebbi (Director, Center for Computational Science) Closing Remarks

C.2 Poster Sessions

(P-1) Y. Bar-Yam (New England Complex Systems Institute and Boston University) "Cellular Automata for Massively Parallel Polymer Simulations with Application to 2-D Melts, Gel-Electrophoresis and Polymer Collapse"

(P-2) John Georgiadis (University of Illinois) "Lattice Boltzmann Simulations of Steady Inertial Flow in Randomly Packed Beds Confined in a Channel"

(P-3) Somalee Datta (Boston University) "Development of Structure in Lattice-Gas Models with Kac Potential Interaction"

(P-4) D. Grubert (Hannover) "Effective Parameters from Simulating Tracer Dispersion in Fractures by Means of the Lattice-BGK Method"

(P-5) Shuling Hou (LANL) "Evaluation of two lattice Boltzmann models for multiphase flows"

(P-6) Jian Huang (Drexel University) "A Thermal LBGK model for High Mach Number and Large Density and Temperature Differences"

(P-7) Antal Karolyi (Budapest) "Lattice Gas Simulations of Granular Media"

(P-8) Robert Maier (Army High Performance Computing Research Center) "Accuracy of the Lattice Boltzmann Method"

(P-9) Colin Marsh (Oxford) "Theoretical Developments in Dissipative Particle Dynamics"

(P-10) Andrew Emerton (Oxford) "Shear Induced Isotropic-to-Lamellar Transition in Lattice-Gas Automata Model of Amphiphilic Systems"

(P-11) Akira Tsumaya (University of Tokyo) "Immiscible lattice gas with long-range interaction"

(P-12) Alexander Wagner (Oxford) "Lattice Boltzmann simulations of two-dimensional deformable drops"

(P-13) Yanan Wu (University of Western Ontario) (TBA)

(P-14) Feng Xu (Drexel) "The Lattice Boltzmann Simulation and Astrophysical Challenge to Hydrodynamics"

(P-15) Anatoly Malevanets (University of Toronto) "Phase Transitions in a Microscopic Model for FitzHugh-Nagumo Kinetics"

(P-16) Patrick Warren (Unilever) "Lattice Boltzmann simulations of electroviscous phenomena"

(P-17) Eirik Flekkoy (Oslo) "Bubbles in Sand: A Lattice Boltzmann Model for Granular Flow"

(P-18) Raissa D'Souza (MIT) "Scaling of Roughness in Thin Films Grown by Ballistic Deposition"

D Proceedings of the Sixth International Conference on Discrete Models for Fluid Mechanics

This is the table of contents of the Proceedings of the Sixth International Conference on Discrete Models for Fluid Mechanics. These proceedings have been published as a special issue (Vol. 8, No. 4, August, 1997) of the *International Journal of Modern Physics C.*

CONTENTS